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Simulation of random fields for stochastic finite element analysis

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ABSTRACT: An increasing attention is paid to probabilistic treatment of both commercial and academic research finite element codes. Computational demands are often high, especially in case of nonlinear problems. Simulation of random fields is the fundamental task in stochastic finite element method (SFEM). There are many techniques available nowadays, but for computationally intensive problems (typically nonlinear FEM calculations) we are constrained by small number of Monte Carlo type simulations we can afford. The paper proposes a method which combines the spectral decomposition of covariance matrix and improved Latin Hypercube Sampling (LHS). Paper tackles some extremely important aspects of random fields simulation for SFEM with small number of simulations at satisfactory accuracy: improvements to both basic statistical moments and autocorrelation structure of simulated random field. All these aspects are important for computational efficiency, robustness and accuracy in SFEM.

1 INTRODUCTION

Stochastic finite element method (SFEM) had facilitated the use of random fields in computational mechanics. Many material and other parameters are uncertain in nature and/or exhibit random spatial variability. Efficient simulation of random fields for problems of stochastic continuum mechanics is in the focus of both researchers and engineers. Achievements in stochastic finite element approaches increased the need for accurate representation and simulation of random fields to model spatially distributed uncertain parameters.

The spatial variability of mechanical and geometrical properties of a system and intensity of load can be conveniently represented by means of random fields. Various methods have been developed for the representation and simulation of random fields utilized within the framework of SFEM e.g. (Vanmarcke et al. 1986, Yamazaki et al. 1988, Schuëller et al. 1990, Liu et al. 1995) and many others.

The computational effort in reliability problem is proportional to the number of random variables, therefore it is desirable to use small number of random variables to represent a random field. Simulation of the random field by a few random variables is especially suitable for problems where theoretical failure probability should be calculated. It enables an efficient use of advanced simulation techniques based on *importance sampling* (Brenner 1991). To achieve this goal, the transformation of the original random variables into a set of uncorrelated random variables can be performed through an eigenvalue orthogonalization procedure (Schuëller et al. 1990, Liu et al. 1995). It is demonstrated that a few of these uncorrelated variables with largest eigenvalues are sufficient for the accurate representation of the random field (Zhang and Ellingwood 1995).

Monte Carlo type generation of random fields is based on combination of orthogonal transformation of covariance matrix (*spectral decomposition*) and LHS. This combination has been recently proposed e.g. Novák et al. (2000) or Olsson and Sandberg (2002).

2 ORTHOGONAL TRANSFORMATION OF COVARIANCE MATRIX

Suppose that a spatial variability of random parameter is described by the Gaussian random field $a(\boldsymbol{x})$, $\boldsymbol{x} = (x, y, z)$ is the vector coordinate which determines the position on the structure. Numerical analysis requires a discrete representation of random field. A continuous field $a(\boldsymbol{x})$ is described by discrete values $a(\boldsymbol{x}_i) = a(x_i, y_i, z_i)$, where $i = 1, \ldots, N$ denotes the discretization point.

The autocorrelation function of the spatial homogeneous random field is supposed to be a function of the distances between two points $|\Delta x|$, $|\Delta y|$ and $|\Delta z|$. The following commonly used exponential form of an autocorrelation function is considered (written in one dimension, for random process):

$$R_{aa}(\Delta x) = \sigma^2 \cdot exp\left[-\left(\frac{|\Delta x|}{d_x}\right)^{pow}\right] \qquad (1)$$

in which d_x is positive parameter called *correlation length* and σ is the standard deviation of the random field. With increasing d_x a stronger statistical correlation of a parameter in space is imposed and opposite. Note, that an isotropic autocorrelation function has all correlation lengths identical, $d_x = d_y = d_z$. The power pow is usually two which leads to well known *bell-shaped* (or squared exponential) autocorrelation function.

When the finite element method is used, the structure is divided into an appropriate number of finite elements of small sizes. The size of each finite element must be small enough from the material property variability (correlation length), as well as from the stress/strain gradient point of view. It must be small enough so that the values of random field can be considered approximately constant within each element (or vicinity of an integration point). Note that generally the discretization mesh of random field mesh and finite element mesh may be different. Consider the fluctuating components of the homogenous random field, which is assumed to model the material property variation around its expected value. Then the N values, $a_i = a(\boldsymbol{x}_i)$, are random with zero mean and autocorrelated. $\boldsymbol{x}_i$ is the location of the centroid of element i or integration point (depending on the discretization of random field). Their correlation characteristics can be specified in term of the covariance matrix C_{aa}, whose ij-component is given by:

$$c_{ij} = Cov[a_i a_j] = R_{aa}(\Delta \boldsymbol{x}_{i,j}) \qquad (2)$$

The random variables can be transformed to the uncorrelated normal form by solution of an eigenvalue problem, e.g. (Schuëller et al. 1990, Liu et al. 1995):

$$\boldsymbol{C}_{\mathbf{XX}} = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^T \qquad (3)$$

where $\boldsymbol{C}_{\mathbf{XX}}$ is the covariance matrix (obtained by discretization from autocorrelation function; for unit variance, $\sigma^2 = 1$). The matrix $\boldsymbol{\Phi}$ represents the orthogonal transformation matrix (eigenvectors).

The covariance matrix in the uncorrelated space $\boldsymbol{Y}$ is diagonal matrix $\boldsymbol{\Lambda} = \boldsymbol{C}_{\boldsymbol{YY}}$, where the elements of diagonal are the eigenvalues $(\lambda_1, \ldots, \lambda_n)$ of covariance matrix $\boldsymbol{C}_{\mathbf{XX}}$.

Usually, not all eigenvalues have to be calculated and considered for the next step (simulation of random variables) as the fluctuations can be described almost completely by a few random variables. This can be done by arranging the eigenvalues in descending order, calculating the sum of the eigenvalues up to the i-th eigenvalue and dividing it by trace of $\boldsymbol{\Lambda}$. This criterion for reduction is very natural as it is based on control of variability captured by reduced set of random variables. Eigenvalue matrix of covariance matrix of $\boldsymbol{Y}$ contains variances of random variables. They are equivalent to eigenvalues, only the largest eigenvalues are dominating and should be used. The question "how many?" can be answered by calculating the ratio of contribution of eigenvalues to the overall variability of field. Note that the selection is a compromise solution: Less variables is used less variability is captured. The reduction results generally to simulation of random field which have variance smaller than required. A certain underestimation of this statistics will always occur.

The reduction of number of random variables in fact depends on relationships between total dimensions and discretization of the structure (model) and given correlation lengths. If the random properties of closely adjacent elements are correlated, the original (full) set of random variables can be represented by a smaller number of uncorrelated random variables. If the correlation length is large (with respect to dimension of structure and discretization) the reduction is progressive. In limiting case when correlation length approaches infinity, the result is that random field can be represented by one random variable only (random field is equivalent to random variable). Opposite, if correlation length approaches zero, no reduction is possible and all random variables have to be involved for proper representation of random field. Example of description of the randomness by the most important random variables is given in Fig. 1. And in addition to, reduction could be a corollary of a truncation error in solution of eigenvalues of $\boldsymbol{C}_{\mathbf{XX}}$. In cases when correlation lengths are comparable to total dimensions of heavily discretized model the solution of eigenvalues of assembled covariance matrix results in a few dominant eigenvalues and many small eigenvalues which can be neglected.

These aspects are illustrated in Fig. 1 where the sum of eigenvalues divided by trace (portion of normalized variability expressed in percentage) is plotted vs. number of random variables used for representation. We considered a structure of length 10 m (e.g. beam) divided into 128 discretization points associated with finite elements ($N = 128$). For univariate Gaussian random process with zero mean, unit variance and squared-exponential autocorrelation function, two values of correlation length are considered in order to show the influence of this parameter, $d = 0.1$ m and $d = 1$ m. It can be seen that in order to cap-

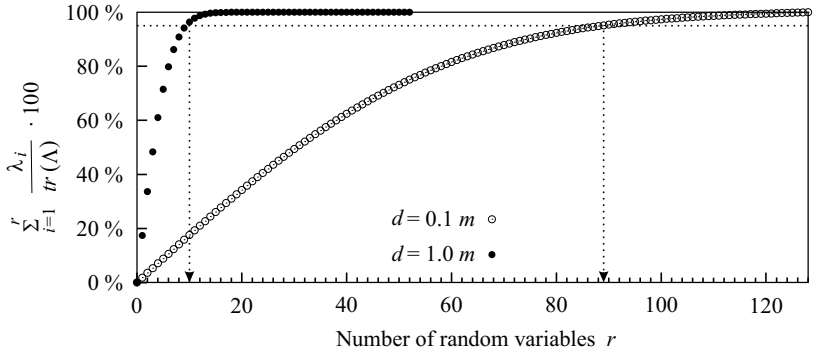

Figure 1: Reduction of number of random variables based on normalized variability.

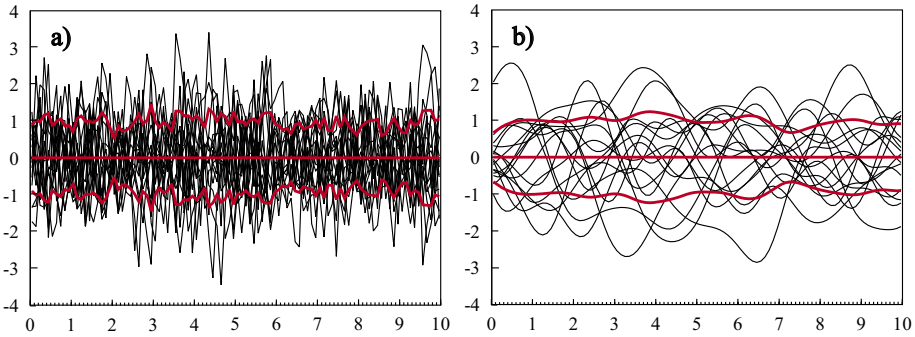

Figure 2: Random field realizations for correlation length a) $d = 0.1$ m; and b) $d = 1$ m. Estimated *mean processes* and $\pm$ *standard deviations* are plotted.

ture the variability of random field, smaller number of random variables r is needed in case of larger correlation length. For example, in order to simulate 95 % of variability we need only 10 largest eigenmodes in case of $d = 1$ m; but for $d = 0.1$ m we need 89 of them. Random field realizations are illustratively shown in Fig. 2 for $N_{Sim} = 16$ simulations only.

Let the chosen number of important dominating random variables by eigenvalue analysis be N_V. Now, the eigenvector matrix $\boldsymbol{\Phi}$ denotes the reduced eigenvector matrix containing only the respective eigenvectors to the N_V most important eigenvalues. Then the vector of uncorrelated Gaussian random variables $\boldsymbol{Y}^T = [Y_1, Y_2, \ldots, Y_{N_V}]$ can be simulated by a traditional way (Monte Carlo simulation). The random variables of vector $\boldsymbol{Y}$ have mean zero and standard deviation $\sqrt{\lambda_1}, \sqrt{\lambda_2}, \ldots, \sqrt{\lambda_{N_V}}$. The transformation back into correlated space yields the random vector $\boldsymbol{X}$ by the relation:

$$\boldsymbol{X} = \boldsymbol{\Phi Y} \tag{4}$$

As already mentioned, the procedure enables significant reduction of uncorrelated random variables for representation of random field especially for higher values of correlation length. These random variables can be simply generated by plain MCS, representation of random field is formed via formula (4).

There are two major computational burdens associated with the method:

1. *Solution of eigenvalue problem*. This may be seen as a serious drawback of the technique for large SFEM system. But such initial computational effort is rewarded later at the step of Monte Carlo simulation resulting in efficient and transparent technique.
2. *Simulation of uncorrelated random variables.* The impact of accuracy in simulation of random variables is studied in the following.

The main advantage of this approach is that advanced simulation techniques based on the concept of importance sampling can be used for reliability calculations because these techniques can usually work efficiently under the set of limited number of random

variables. The possibility of determination of theoretical failure probability with a good numerical accuracy is then guaranteed.

The vector of uncorrelated Gaussian random variables $\boldsymbol{Y}^T = [Y_1, \ldots, Y_n]$ can be simulated by a traditional way (Monte Carlo simulation). LHS can be used for simulation of $\boldsymbol{Y}$ (Novák et al. 2000). This paper clarifies impact of accuracy of correlation structure of samples as well as significance of accuracy of sampling scheme itself. Next comment is therefore devoted to LHS methodology. Later, LHS is utilized by authors for simulation of statistically uncorrelated random variables with Gaussian distribution and compared to classical Monte Carlo simulation (Vořechovský and Novák 2003).

3 LATIN HYPERCUBE SAMPLING UTILIZATION

Majority of papers on LHS is focused on the level of random variables and LHS is rarely employed for random fields simulation in SFEM. The aim of this section is to repeat the possibility of improvement of the method based on orthogonal transformation of covariance matrix for random field simulation and to show some new improvements to the method. The approach is based on utilization of stratified sampling technique LHS for simulation of dominating uncorrelated random variables. The result is that only a few random variables and quite small number of simulations is necessary for accurate representation of a random field. This should be proved at least numerically. The methodology for an assessment of error of simulations is described in section 4, numerical examples inclusive. A comparison with classical Monte Carlo simulation (MCS) reveals the superior efficiency and accuracy of the method. A parametric studies focused on the quality of simulated random fields (target statistical parameters and simulated statistical characteristics of random field) are presented later. An emphasize is given to the region of very small numbers of simulations (tens, hundreds) which is particularly important for SFEM analysis of complex computationally intensive problems.

Small number of simulations can be used for acceptable accuracy using some stratified sampling, one often used alternative is LHS technique. This technique belongs to the category of advanced simulation methods (McKay et al. 1979, Iman and Conover 1980, Iman and Shortencarier 1984).

When any method for random field simulation is used it is required that the statistical characteristics of the field generated should be as close as possible to the target statistical parameters. Generally, the mean values, standard deviations, correlation and spectral characteristics (we will use the common term "statistics") cannot be generated with absolute accuracy. Basic information about random field is captured by its second moment characteristics, i.e. the mean function μ and the covariance function C_{aa}.

Here should be tackled some extremely important aspects of random fields simulation for stochastic finite element analysis (SFEM): Spurious correlation reduction, a restriction resulting from Cholesky decomposition of covariance matrix, orthogonal transformation of covariance matrix (called sometimes *spectral decomposition*) and the utilization of Latin hypercube sampling (LHS) for random fields simulation. All these aspects are important for computational efficiency, robustness and accuracy in SFEM. A superiority of LHS was already showed by many researchers, e.g. (Novák et al. 2000, Bucher and Ebert 2000, Olsson and Sandberg 2002) and others. A practical consequence is using small number of simulations of random field to achieve satisfactory accuracy. In spite of these achievements some arising questions remained not answered and remarks should be done.

3.1 *Classification of sampling schemes*

There are three different method to diminish spurious correlation available nowadays: Method based on Cholesky decomposition of covariance matrix, (Iman and Conover 1982); Single-switch optimization scheme, (Huntington and Lyrintzis 1998); Method based on simulated annealing due to Vořechovský and Novák (2002) which will be used in the following.

Hypothetically, there are 6 combinations.

- crude Monte Carlo simulation denoted "MCS";
- LHS under original scheme denoted "LHS-median", (McKay et al. 1979);
- LHS under improved scheme denoted "LHS-mean", (Huntington and Lyrintzis 1998), an alternative described later on.

These schemes can be applied in two alternatives:

- No attention paid to spurious correlation (SC);
- Spurious correlation diminished (SCD)

There are 6 combinations, cases with SC and SCD, which are sampled by MC, LHS-median and LHS-mean. What is the best alternative? Naturally, the quality of sampling schemes can be intuitively predicted even without numerical experiment, e.g. combination (MCS) and (SC) should definitely belong to worst case and combination of (LHS-mean) and (SCD) should be the most efficient. Note, that in case of random field simulation using the orthogonal transformation of covariance matrix, the quality of sampling is influenced by criterion for a reduction of number of random variables. A proper error assessment based on numerical experiment is therefore the most objective method for qualitative assessment of sampling schemes listed above.

The quality of generated random field is a primary task and should be tested first. The approach for error assessment can be elaborated in a similar way to as the general error assessment procedure due to (Novák et al. 1995, Novák et al. 2000).

3.2 *Improvements to autocorrelation structure*

Sampling scheme of LHS can be represented by matrix $\boldsymbol{Y}$, where samples are in N_{Sim} rows and N_V columns related to random variables (N_V is number of input variables). During classical LHS sampling a spurious (random) correlation can be introduced between random variables (columns in $\boldsymbol{Y}$). It can happen especially in case of very small number of simulations N_{Sim} (tens), where the number of interval combination is rather limited.

The imposition of prescribed statistical correlation into sampling scheme can be understood as an optimization problem: The difference (expressed by a matrix norm E) among prescribed $\boldsymbol{K}$ and generated $\boldsymbol{S}$ correlation matrices should be as small as possible. The methodology for reduction of spurious correlation based on optimization technique *Simulated Annealing* (SA) is proposed and thoroughly described by Vořechovský and Novák (2002); technique has a great consequence: There is no restriction concerning number of simulations n. Number of simulations can be extremely low as covariance matrix of $\boldsymbol{Y}$ does not have to be positive definite. There is a penalty for this advantage: Spurious correlation can be diminished only until certain limit.

What are the consequences of spurious correlation to autocorrelation function variability of simulated random fields? The study has been performed with a random process from the example in section 2 with autocorrelation length $d = 1$ m and for two numbers of simulations – an error assessment based on samples simulations from population is described later. From all 128 random variables only 52 has been used after orthogonalization procedure to represent random field (the smallest eigenvalue taken into account was $1 \cdot 10^{-15}$, which represents a random variable with negligible standard deviation). The results are shown in Fig. 3, mean values and the scatterband represented by mean $\pm$ standard deviation of autocorrelation function is plotted. Figure 3a) shows the result for $N_{Sim} = 32$, spurious correlation is not diminished (LHS-mean-SC). It is obvious that capturing of target autocorrelation function is weak and the scatterband is large. The explanation is clear, using only $N_{Sim} = 32$ leads to large both norms (E_{max} and $E_{overall}$) used as the objective function to be minimized in Simulated annealing algorithm (Vořechovský and Novák 2002). Only a slight improvement can be seen if spurious correlation is diminished (LHS-mean-SCD), Fig. 3b). When N_{Sim} increases to 64, capturing of autocorrelation function is better, Fig. 3c), d). Note that now the alternative with diminished spurious correlation by SA resulted in excellent function capturing with very small variability, see figure 3d). This fact corresponds with both norms which are in case d) very small. It can be seen that the spurious correlation at the level of simulation of independent random variables influences negatively the autocorrelation function. These illustrative figures also clearly indicate that norms used as objective functions in Simulated Annealing algorithm (Vořechovský and Novák 2002) can be interpreted as a qualitative prediction of resulting quality of autocorrelation structure.

3.3 *Improvements to sampling of random variables*

The classical approach of LHS is to use centroids of layers on distribution function to obtain realizations $y_{i,t} = F_i^{-1}[(t + 0.5/n)]$ a method denoted "LHS-median". Huntington and Lyrintzis (1998) showed that this approach gives samples with a mean close to desired one, but sample variances can be significantly different. They proposed sampling scheme (also used by Keramat and Kielbasa (1997), where the representative value of each layer on distribution function should be chosen as probabilistic mean of corresponding disjunct interval "LHS-mean":

$$y_{i,t} = n \int_{z_{i,t-1}}^{z_{i,t}} y \cdot f_i(y)\, dy \tag{5}$$

where f_i is PDF of variable Y_i. Integration limits define boundaries of equiprobable intervals:

$$z_{i,t} = F_i^{-1}\left(\frac{t}{n}\right) \tag{6}$$

where F_i is CDF of variable Y_i. This sampling gives arithmetic mean equal to the desired one (sampling follows the definition of mean value) and variability of sample set much closer than that of the current technique.

4 ERROR ASSESSMENT OF RANDOM FIELDS SIMULATION

4.1 *The concept of assessment*

The quality of simulated random field is a primary task and should be tested first, before any application with physical computational model. Some samples of random fields for a parameter are simulated from the population parameters. A certain statistics of the particular simulation may be very close to or quite far away from the value of corresponding target parameter. When the seed of the pseudo-random number generator is changed, other random fields are generated and other values of all sample statistics are naturally obtained. Therefore, each of these statistics can

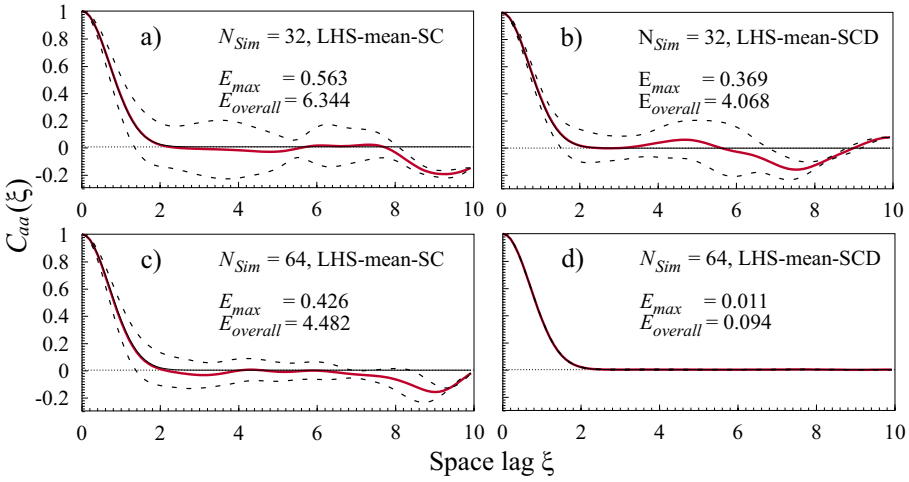

Figure 3: Scatterband of autocorrelation function $C_{aa}(\xi)$ for $N_{Sim} = 32$: a) LHS-mean-SC; b) LHS-mean-SCD; and $N_{Sim} = 64$: c) LHS-mean-SC; d) LHS-mean-SCD.

be considered as a random variable with some mean value and variance. The simulation technique is considered as best one which gives an estimated mean value of the statistics very close to the target mean value and also closest to zero variance of the statistics. In our case of zero mean value and unit variance of random field (basic target statistical parameters) we expect to get estimated mean around zero and variance around one.

The assessment can be done by performing more runs of the same simulation process with a different random setting of the seed of pseudo random number generator. Thus samples are artificially generated from the population in this way. Procedure can be described as follows (for one particular run):

- N_{Sim} simulations of random field are performed with initial random seed setting and prescribed parameters;
- Statistics are evaluated from N_{Sim} generated realizations of the random field over all N discretization points (capturing also the ergodicity as the basic property of random field) *mean* $\overline{a_s}$ and *standard deviation* σ_{a_s} are evaluated.
- Correlation and spectral characteristics are estimated and compared to the target autocorrelation function or power spectral density.

The procedure itemized above is repeated N_{run} times, each time with different initial random setting of the seed. Naturally, statistics obtained in each run are different, e.g. different *mean* $\overline{a_s}$ and *standard deviation* σ_{a_s}. As measures of the accuracy of simulation, the mean values and standard deviation are calculated from N_{run} statistics obtained. Symbolically, we assign the following symbols:

- Mean($\overline{a_s}$), Mean(σ_{a_s}) for mean values of *mean* $\overline{a_s}$ and *standard deviation* σ_{a_s}.
- Std($\overline{a_s}$), Std(σ_{a_s}) for standard deviations of *mean* $\overline{a_s}$ and *standard deviation* σ_{a_s}.

If the simulation is successful, then Mean($\overline{a_s}$) $\to 0$, Mean(σ_{a_s}) $\to 1$ and standard deviations Std(.) $\to 0$ (hypothetical limits for $N_{Sim} \to \infty$).

4.2 *Numerical results*

For the numerical study, let us consider the univariate random process from section 2. The region of small number of simulations ($N_{Sim} = 8, 16, 32, 64, 128, 256, 512$) has been selected in parametric study – implicitly it was supposed that the superiority of LHS should appear for small number simulations (tens, hundreds). Number of runs $N_{run} = 30$ was selected for estimation of statistics. So the random fields had to be simulated $N_{run} \times N_{Sim}$ times for a statistics of interest.

The following alternatives have been selected for the error assessment: MCS-SC, MCS-SCD, LHS-median-SC, LHS-median-SCD, LHS-mean-SC and LHS-mean-SCD. The results are plotted in Fig. 4.

Mean value: An ability to simulate *mean value* of random field is excellent in all alternatives of LHS

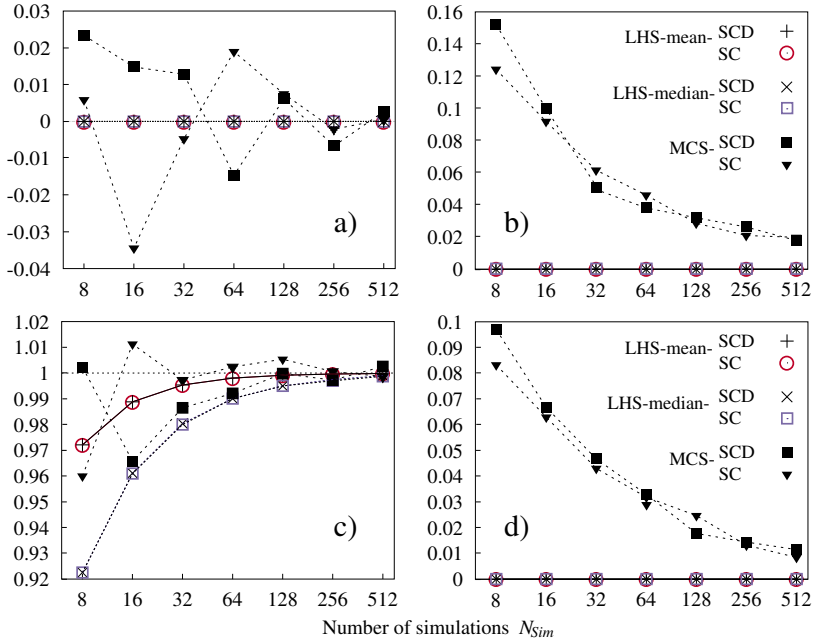

Figure 4: Statistics of *mean* and *standard deviation* ($d = 1$ m): a) mean of *mean*; b) standard deviation of *mean*; c) mean of *standard deviation*; d) standard deviation of *standard deviation*

(figures a) and b)), even for very low number of simulations. This ability is rather poor in case of MCS, mean value of *mean* fluctuates and standard deviation of *mean* is high in comparison to LHS (around the order 10^{-18} for LHS alternatives, which is just a noise due to numerical inaccuracy).

Standard deviation: The ability to simulate *standard deviation* of random field is documented in figures c) and d). Again, capturing of this statistics is "random" in case of MCS, standard deviation of *standard deviation* is high in comparison to LHS. LHS-median underestimates mean value of *standard deviation* (figure c)) for low number of simulations. The capability of improved sampling scheme LHS-mean is much better and convergence to target statistic (unit standard deviation) is faster. This is a general feature of LHS tested at the level of random variables.

An important fact is documented: There is no significant difference between alternatives SC and SCD in case of MCS, LHS-median and LHS-mean sampling schemes. Both LHS methodologies generally prescribes *mean value* in section (discretization point) of a field, but variability (*standard deviation*) in section is better for LHS-mean sampling.

Diminishing spurious correlation has small influence on these basic statistics of random field (in our study statistics of random fields are "smeared" lengthwise, but an impact of spurious correlation could remain in sections of random field realizations). In most cases differences are negligible and points coincide in presented figures. As was shown above, a spurious correlation influences negatively the autocorrelation structure of random field. Note, that if we construct statistics presented in Fig. 4 for different correlation length of the field, similar trends will be obtained.

5 CONCLUSIONS

It has been shown that a spurious correlation influences significantly the scatter of autocorrelation function of simulated random fields. A decrease of scatter-band is influenced by the possibility to diminish the spurious correlation. The method for diminishing spurious correlation based on stochastic optimization method SA appeared to be robust and efficient for random field simulation. This possibility is limited in case of very small number of simulations (with respect to number of random variables representing random field). A clear indication of this limitation is the fulfillment of norms used as objective functions in SA to diminish spurious correlation.

The quality of simulated random fields should be

assessed by usage of both basic statistics (mean value and standard deviations) applied for simulated mean and standard deviation. An error assessment has been performed for six alternatives of sampling schemes. The best performance, ie. the convergence to target values of statistics with low variability has been achieved in case of LHS approach with improvement (LHS-mean). Diminishing spurious correlation does not influence the capturing of these statistics but does influence significantly realization of autocorrelation function of random field.

The superior efficiency of LHS and correlation control is confirmed. But attempt has been done to show better the role of correlation control – diminishing spurious correlation in random field simulation and importance of sampling schemes for simulation of uncorrelated random variables.

The proposed small-sample simulation of random fields is utilized for probabilistic nonlinear fracture mechanics modeling of concrete structures (Novák et al. 2005) and in the context of simulation of random strength field of fibers for multifilament yarns (Vořechovský and Chudoba 2005).

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